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- Weis, P., O. Hampe, S. Gilb and M.M. Kappes, Metastability of isolated platinum and palladium tetrahalide dianions and the role of electron tunneling 321 (2000) 426
- Weitz, A., see Strassner, Th. 321 (2000) 459
- White, J.O., see Zhu, A. 321 (2000) 394
- Woltering, M. and M. Markus, Riddled basins in a model for the Belousov-Zhabotinsky reaction 321 (2000) 473
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- Yates Jr., J.T., see Kuznetsova, A. 321 (2000) 292
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- Yu, H.-G., S. Andersson and G. Nyman, A generalized discrete variable representation approach to interpolating or fitting potential energy surfaces 321 (2000) 275
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- Zhang, R.Q., K.L. Han, R.S. Zhu, C.S. Lee and S.T. Lee, Ab initio/Rice-Ramsperger-Kassel-Marcus approach to carbon nitride formation: CH_3NH_2 decomposition 321 (2000) 101
- Zhao, X., see Carravetta, M. 321 (2000) 205
- Zhong, S. and H. Xin, Noise-induced oscillations and internal stochastic resonance in a model of excitable biomembrane 321 (2000) 309
- Zhou, M., see Chen, M. 321 (2000) 498
- Zhu, A., B. Wang, J.O. White and H.G. Drickamer, The effect of high pressure and controlled stretching on the intramolecular twist of *p*-N-N-dimethylaminobenzylidenemalononitrile in polyvinylacetate and polyvinylchloride 321 (2000) 394
- Zhu, R.S., see Zhang, R.Q. 321 (2000) 101
- Zhu, Y., see Qiao, Z. 321 (2000) 504

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